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Wang-Landau Simulations of Adsorbed and Confined Lattice Polymers

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Abstract

We demonstrate how Wang-Landau simulations may be used in an efficient manner to investigate the statistical mechanics of lattice polymers adsorbed at a planar surface, and confined in slit geometry between two parallel surfaces. For nearest neighbour interactions, we show that one or two Wang-Landau simulations, recording the density of states as a function of numbers of internal contacts and of surface beads, are sufficient to give a full description of both of these situations. Moreover, the efficiency of the simulations is improved by never having to reject moves due to overlap with the surface, and the limit of infinite slit height may be handled easily. The proposed "wall-free" methods have already been applied to homopolymers and heteropolymers (lattice peptides using the HP model) on a uniform surface, as well as regularly patterned surfaces, and could easily be generalized to surfaces with structure.

Keywords:

1. Introduction

This paper is motivated by the current interest in Monte Carlo (MC) simulations of simple lattice models of polymers and peptides, with interactions between nearest-neighbour beads, concentrating on their behaviour near adsorbing surfaces. Although lattice models are very simple, they contain some of the essential physics and chemistry of the problem, especially the problem of locating minimum-energy folded structures. The HP model of lattice peptides [1], for instance, has been described as the "Ising model of protein folding" [2]. This has been a fruitful area for the development of accelerated simulation methods in recent years [3–16]. The essential idea behind the current work has been presented already in the context of the HP model [17, 18] and related work on confined ring polymers will appear elsewhere [19].

2. The Model

For illustrative purposes we adopt the model of a single unbranched homopolymer of L beads on a simple cubic lattice. If a given internal conformation of the polymer Γ has n_Γ nearest neighbour contacts, each of energy $-\epsilon$, then the internal energy is given by $-n_\Gamma\epsilon$. In addition we consider interactions between the polymer and a planar surface, or two identical planar surfaces separated by a distance H, once again involving only nearest-neighbour lattice sites. The strength of the interaction will be denoted $-\sigma$ and the total number of surface-interacting beads in the peptide, in any internal state Γ, is s_Γ. Accordingly the total energy is $E_\Gamma = -n_\Gamma\epsilon - s_\Gamma\sigma$. We note that the extension to the HP model is easily handled by counting only those types of bead that interact with each other, and with the surface.

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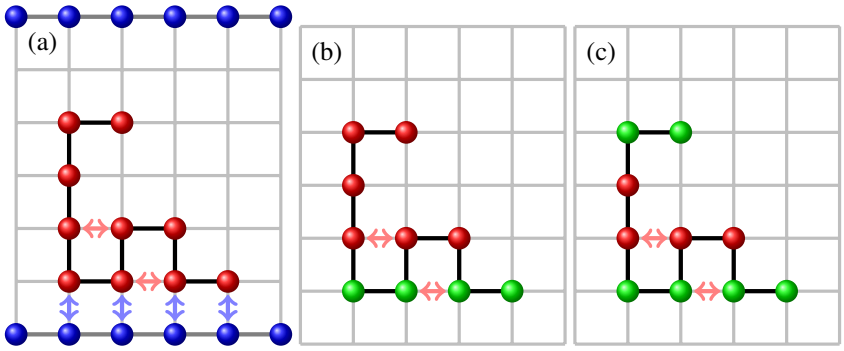

Figure 1: Schematic of wall-free simulation approach. (a) Conventional simulation in slit geometry, counting internal contacts (red) and contacts with surface beads in the walls (blue). (b) Simulation counting internal contacts (red) and beads on the bottom surface of the polymer (green), determining $\mathbb{W}_1(n, s_1)$. (c) Simulation counting internal contacts (red) and beads on both the top and bottom surfaces of the polymer (green), determining $\mathbb{W}_2(n, s_{1\&2})$.

For our purposes, it is convenient to define the positional coordinate of the peptide as

$$(X, Y, Z) = (\min(\{x_i\}), \min(\{y_i\}), \min(\{z_i\}))$$

where (x_i, y_i, z_i) are the coordinates of monomer bead i. The internal state Γ of the peptide is defined with reference to this position. The lower surface (wall) occupies the plane $z = 0$. Polymers are excluded from the region $Z \leq 0$; those with $Z = 1$ interact with the surface (i.e. the lower surface, if there are two); states with $Z > 1$ do not. If a second confining surface is introduced, occupying the plane $z = H + 1$, this defines a slit of height H, i.e. H planes $z = 1, 2, \ldots H$, that may, in principle, be occupied by monomer beads. Let us define the height of a polymer in state Γ, h_Γ, as the number of z-planes occupied by beads: $1 \leq h_\Gamma \leq L$ for the current model. A polymer with coordinate Z and internal state Γ, occupies planes $Z, Z + 1, \ldots, Z + h_\Gamma - 1$. Then, states with $Z \leq H - h_\Gamma$ do not interact with the upper surface, those with $Z = H - h_\Gamma + 1$ may interact with it, and those with $Z > H - h_\Gamma + 1$ are forbidden. We shall consider situations in which the upper and lower surfaces are both attractive, i.e. have nearest-neighbour interactions of strength σ with the polymer beads; in which they both have zero interaction energy, and solely impose the confinement condition by steric exclusion; and in which there is one surface of each type.

We shall take the surface to be uniform, so the X and Y coordinates are not relevant, and can be dropped. We note in passing that it is straightforward to extend to treatment to patterned surfaces, where X and Y become relevant modulo the periodicity of the pattern of adsorption sites in the surface. Periodic boundary conditions are not needed in the simulations, as the aim is to simulate a single molecule only.

3. Confinement

For a single polymer chain in a slit of height H, the density of states $\mathbb{W}_H(n, s)$ may be expressed as a function of the number of internal contacts, and surface contacts (with one or both walls). This will include a summation over all the Z coordinates that are consistent with the specified values of n and s. Given this function, it will be possible to construct a canonical partition function

$$\mathbb{Q}_H(T) = \sum_{n,s} \mathbb{W}_H(n, s) \mathrm{e}^{+\beta n \epsilon} \mathrm{e}^{+\beta s \sigma} \tag{1}$$

where $\beta = 1/k_\mathrm{B}T$, for the molecule in the slit. The situation is illustrated schematically in Figure 1(a). As we shall see, the procedures used to obtain these functions will also be sufficient to give a full description of adsorption at a single surface.

3.1. Two Attractive Surfaces

We consider conducting at most *two* Wang-Landau simulations [20, 21]. The first determines the density of states $\mathbb{W}_1(n, s_1)$ where n is the number of internal contacts and s_1 the number of beads in the lowest surface layer (i.e. the number of beads for which $z_i = Z$). The simulation proceeds by conducting Monte Carlo moves of the lattice polymer, using any desired move set, in the usual way, refining the estimate of $\mathbb{W}_1(n, s_1)$ until, hopefully, convergence is achieved. We typically use "pull moves" in this context [3, 17, 19], but note that recently it has been shown that there is a significant advantage in supplementing these by connectivity-altering moves [14]. No direct account is taken of interactions or exclusions due to the walls; the aim is solely to obtain the relative numbers of internal states available for each specified pair of values (n, s_1). This is illustrated schematically in Figure 1(b). At the same time, the probability distribution functions for height h, $p_1(h|n, s_1)$, are accumulated, for each pair (n, s_1). At the end of the simulation, these functions are normalized such that $\sum_h p_1(h|n, s_1) = 1$ for each (n, s_1). This avoids the necessity of attempting to determine a three-dimensional Wang-Landau density of states; effectively we may write $\mathbb{W}_1(n, s_1, h) = p_1(h|n, s_1)\mathbb{W}_1(n, s_1)$.

The second Wang-Landau simulation determines the density of states $\mathbb{W}_2(n, s_{1\&2})$ where n is once more the number of internal contacts and $s_{1\&2} = s_1 + s_2$ is the *sum* of the number of beads in the lowest *and* uppermost surface layers (i.e. s_1 is the number of beads for which $z_i = Z$ and s_2 is the number for which $z_i = Z + h_\Gamma - 1$). For the case $h_\Gamma = 1$, this involves double-counting the beads, i.e. $s_{1\&2} = 2L$. This is illustrated schematically in Figure 1(c). Once more, a probability histogram for heights $p_2(h|n, s_{1\&2})$ is accumulated and normalized, allowing us to use the formula $\mathbb{W}_2(n, s_{1\&2}, h) = p_2(h|n, s_{1\&2})\mathbb{W}_2(n, s_{1\&2})$.

Both these simulations give independent estimates of the density of states resolved by internal contacts alone, namely

$$\mathbb{W}_0(n) = \sum_s \mathbb{W}_1(n, s) = \sum_s \mathbb{W}_2(n, s) \,,$$

which could be used to calculate the internal partition function of the isolated polymer molecule. Bearing in mind that each Wang-Landau simulation determines $\mathbb{W}$ only to within a multiplicative constant, it is important for what follows that $\mathbb{W}_1$ and $\mathbb{W}_2$ are normalized relative to each other, so as to be consistent with the above equation. (Of course, $\mathbb{W}_0$ could also be determined independently, in which case it is important that all three quantities are normalized consistently). In a similar way, the height probability distribution, $p_0(h|n)$, irrespective of surface contacts, may be obtained by summing $p_1(h|n, s_1)$ over s_1, or $p_2(h|n, s_{1\&2})$ over $s_{1\&2}$, or by calculating directly in a separate simulation of $\mathbb{W}_0$.

The calculation of $\mathbb{W}_H$ is now accomplished by simply summing the states available for each value of Z. For the slit with two identical attractive surfaces, this sum becomes

$$\mathbb{W}_H(n, s) = p_2(H|n, s)\mathbb{W}_2(n, s) + 2\sum_{h=1}^{H-1} p_1(h|n, s)\mathbb{W}_1(n, s) + \delta_{s0}\sum_{h=1}^{H-2}(H - h - 1)p_0(h|n)\mathbb{W}_0(n) \,. \tag{2}$$

The first term counts all states that are in contact with both surfaces, for which the height is exactly $h = H$; this term is zero if $H > L$. The second term counts all states in contact with just one surface: heights up to and including $H - 1$ are allowed; the term is omitted if $H = 1$. The factor 2 in this term accounts for the two positions that allow contact with the lower and upper surfaces, respectively, and relies on $\mathbb{W}_1$ applying equally well to either surface (by symmetry). The third term counts the states which are not in contact with either wall. It contains the Kronecker delta: $\delta_{s0} = 1$ if $s = 0$ and $\delta_{s0} = 0$ otherwise. Heights up to and including $H - 2$ are allowed; this term is dropped if $H \leq 2$. The factor $(H - h - 1)$ inside the sum counts the number of Z positions that are accessible for each value of h.

Equation (2) is simplified if we define cumulative probabilities $P(h) = \sum_{h'=1}^{h} p(h')$:

$$\mathbb{W}_H(n, s) = p_2(H|n, s)\mathbb{W}_2(n, s) + 2P_1(H - 1|n, s)\mathbb{W}_1(n, s) + \delta_{s0}\left[(H - 1)P_0(H - 2|n) - \sum_{h=1}^{H-2} hp_0(h|n)\right]\mathbb{W}_0(n) \,, \tag{3}$$

where $P(h) = 0$ if $h = 0$, and $P(h) = 1$ if $h \geq L$. The slit partition function, eqn (1), derived from this is

$$\mathbb{Q}_H(T) = \sum_{ns}\Big[p_2(H|n,s)\mathbb{W}_2(n,s) + 2P_1(H-1|n,s)\mathbb{W}_1(n,s)\Big]\mathrm{e}^{+\beta n\epsilon}\mathrm{e}^{+\beta s\sigma} + \sum_n\left[(H-1)P_0(H-2|n) - \sum_{h=1}^{H-2} hp_0(h|n)\right]\mathbb{W}_0(n)\mathrm{e}^{+\beta n\epsilon}\,. \quad (4)$$

Further simplification occurs in the event that the slit height is larger than the maximum height (length) of the polymer. If $H \geq L+2$ then $p_2(H|n,s) = 0$, $P_1(H-1|n,s) = P_0(H-2|n) = 1$, and

$$\begin{aligned}\mathbb{W}_H(n,s) &= 2\mathbb{W}_1(n,s) + \delta_{s0}[H-1-\overline{h}(n)]\mathbb{W}_0(n)\\ \mathbb{Q}_H(T) &= 2\sum_{ns}\mathbb{W}_1(n,s)\mathrm{e}^{+\beta n\epsilon}\mathrm{e}^{+\beta s\sigma} + \sum_n[H-1-\overline{h}(n)]\mathbb{W}_0(n)\mathrm{e}^{+\beta n\epsilon}\end{aligned} \quad (5)$$

where $\overline{h}(n)$ is the average height for polymers having n internal contacts. Note that no knowledge of $\mathbb{W}_2$ is required in this case.

3.2. One Attractive and One Steric Surface

For a slit where the second surface acts only to sterically confine the polymer, without any attractive interactions, the slit density of states also does not require knowledge of $\mathbb{W}_2$:

$$\begin{aligned}\mathbb{W}_H(n,s) &= \sum_{h=1}^{H} p_1(h|n,s)\mathbb{W}_1(n,s) + \delta_{s0}\sum_{h=1}^{H-1}(H-h)p_0(h|n)\mathbb{W}_0(n)\\ &= P_1(H|n,s)\mathbb{W}_1(n,s) + \delta_{s0}\left[HP_0(H-1|n) - \sum_{h=1}^{H-1} hp_0(h|n)\right]\mathbb{W}_0(n)\,,\end{aligned} \quad (6)$$

and the partition function is

$$\mathbb{Q}_H(T) = \sum_{ns} P_1(H|n,s)\mathbb{W}_1(n,s)\mathrm{e}^{+\beta n\epsilon}\mathrm{e}^{+\beta s\sigma} + \sum_n\left[HP_0(H-1|n) - \sum_{h=1}^{H-1} hp_0(h|n)\right]\mathbb{W}_0(n)\mathrm{e}^{+\beta n\epsilon}\,. \quad (7)$$

For slit heights $H \geq L+1$ we get the much simpler formulae

$$\mathbb{W}_H(n,s) = \mathbb{W}_1(n,s) + \delta_{s0}[H-\overline{h}(n)]\mathbb{W}_0(n)\,, \quad \mathbb{Q}_H(T) = \sum_{ns}\mathbb{W}_1(n,s)\mathrm{e}^{+\beta n\epsilon}\mathrm{e}^{+\beta s\sigma} + \sum_n[H-\overline{h}(n)]\mathbb{W}_0(n)\mathrm{e}^{+\beta n\epsilon}\,. \quad (8)$$

3.3. Two Steric Surfaces

The simplest confined system is one in which there are no attractive interactions at all, and the walls just act sterically. In this case, the formulae corresponding to eqns (6) and (7) become

$$\begin{aligned}\mathbb{W}_H(n) &= \sum_{h=1}^{H}(H-h+1)p_0(h|n)\mathbb{W}_0(n) = \left[(H+1)P_0(H|n) - \sum_{h=1}^{H} hp_0(h|n)\right]\mathbb{W}_0(n)\,,\\ \mathbb{Q}_H(T) &= \sum_n\left[(H+1)P_0(H|n) - \sum_{h=1}^{H} hp_0(h|n)\right]\mathbb{W}_0(n)\mathrm{e}^{+\beta n\epsilon}\end{aligned} \quad (9)$$

For slit heights $H \geq L$ these simplify to

$$\mathbb{W}_H(n) = [H+1-\overline{h}(n)]\mathbb{W}_0(n)\,, \quad \mathbb{Q}_H(T) = \sum_n[H+1-\overline{h}(n)]\mathbb{W}_0(n)\mathrm{e}^{+\beta n\epsilon} \quad (10)$$

For obvious reasons, the surface beads do not enter into these equations at all, and a single Wang-Landau simulation determining the one-dimensional density of states $\mathbb{W}_0(n)$, together with $p_0(h|n)$, is all that is needed.

In practice, we find it convenient to determine the two-dimensional function $\mathbb{W}_0(n,h)$ itself using the Wang-Landau method, rather than accumulating $p_0(h|n)$ while determining $\mathbb{W}_0(n)$. However, it is important (as in all Wang-Landau simulations) to monitor the sampling of the chosen variables: in certain circumstances (for instance, very long ring polymers) we found that the transition from $h = 2$ to $h = 1$ was attempted very rarely, due to the infrequency of occurrence of states with $h = 2$ that were capable of conversion (through pull moves) to a completely flat configuration. This was addressed successfully by subdividing the $h = 2$ bins according to the numbers of beads in each layer, ensuring that the distribution of sampled states amongst the sub-bins became flat in the natural operation of the algorithm.

4. Adsorption

In all of the cases discussed in the previous section, the slit height H appears explicitly, and the regularization of the partition function giving thermodynamic quantities which include a translational entropy proportional to $\ln V$ (i.e. $\ln H$) is also easy to see. This was discussed recently for off-lattice models by Möddel et al [15, 16]. Formally, the discussion of adsorption at a single interface relies on allowing H to increase sufficiently that the two walls do not interact, indeed extrapolating such that $H \to \infty$, so that the adsorption system may be considered at equilibrium with a well-defined bulk phase. The forms of eqns (2)–(10), and the fact that quantities in them may be obtained from "wall-free" simulations, lead to the expectation that slit geometry is not necessary to discuss adsorption for the current class of models.

Indeed, this is the case, and two types of "thought" simulation may be conducted to highlight this. Firstly, it is possible to consider a surface of interest at $z = 0$, and define a confining, steric, wall such that it applies to the beads on the lower surface, rather than the upper surface, of the polymer. The molecule may therefore partially extend beyond the steric wall, but it is confined such that at least some part of it lies within the slit. This greatly simplifies the formulae (6) and (7) of the previous section: every internal state Γ has exactly the same set of positions Z accessible to it, of which $Z = 1$ is in contact with the surface of interest, and all the remaining $H - 1$ positions are not. Accordingly, the slit densities of states, and the partition functions derived from them, are simple sums of the kind

$$\mathbb{W}_H(n,s) = \mathbb{W}_1(n,s) + \delta_{s0}[H-1]\mathbb{W}_0(n)\,, \tag{11}$$

$$\mathbb{Q}_H(T) = \mathbb{Q}_1(T) + [H-1]\mathbb{Q}_0(T)\,, \tag{12}$$

where the key partition functions are given by

$$\mathbb{Q}_1(T) = \sum_{n,s} \mathbb{W}_1(n,s)\mathrm{e}^{+\beta n\epsilon}\mathrm{e}^{+\beta s\sigma}\,, \quad \text{and} \quad \mathbb{Q}_0(T) = \sum_{n} \mathbb{W}_0(n)\mathrm{e}^{+\beta n\epsilon}\,. \tag{13}$$

In discussing adsorption, we wish to calculate the number of adsorbed molecules relative to the number in the bulk, far from the surface. Here, "far from the surface" simply means $Z > 1$, i.e. a slit of height $H = 2$ is sufficient! (Recall that we are simulating a single molecule, subject to nearest-neighbour interactions). So, for $H = 2$, we have simply $\mathbb{Q}_H(T) = \mathbb{Q}_1(T) + \mathbb{Q}_0(T)$. The desired ratio is, from the definition of the partition function, $\langle N_{\mathrm{ads}}\rangle/\langle N_{\mathrm{des}}\rangle = \mathbb{Q}_1/\mathbb{Q}_0$. Alternatively we may discuss adsorption in a slit as a function of the chemical potential μ or activity $\lambda = \mathrm{e}^{\beta\mu}$. In the grand canonical ensemble, we can create or remove particles in positions which are adjacent to the surface, in the bulk, or close to the remote wall. For an ideal gas of N non-interacting polymers, the grand partition function may be written for each location Z

$$\mathbb{X}(\lambda,T) = \sum_{N\geq 0} \frac{\lambda^N \mathbb{Q}^N}{N!} = \mathrm{e}^{\lambda\mathbb{Q}} \quad \Rightarrow \quad \langle N\rangle = \lambda\frac{\partial \mathbb{X}(\lambda,T)}{\partial\lambda} = \lambda\mathbb{Q}\,.$$

Irrespective of the details at the remote wall, the adsorption may be discussed by comparing the grand potential $\mathbb{X}_1$, for $Z = 1$ adjacent to the surface of interest, with $\mathbb{X}_0$, for $Z > 1$, in the bulk. This leads to the same result seen earlier, $\langle N_{\mathrm{ads}}\rangle/\langle N_{\mathrm{des}}\rangle = \mathbb{Q}_1/\mathbb{Q}_0$. These quantities are provided directly by the Wang-Landau simulations described earlier: there is no need to actually conduct a simulation in slit geometry.

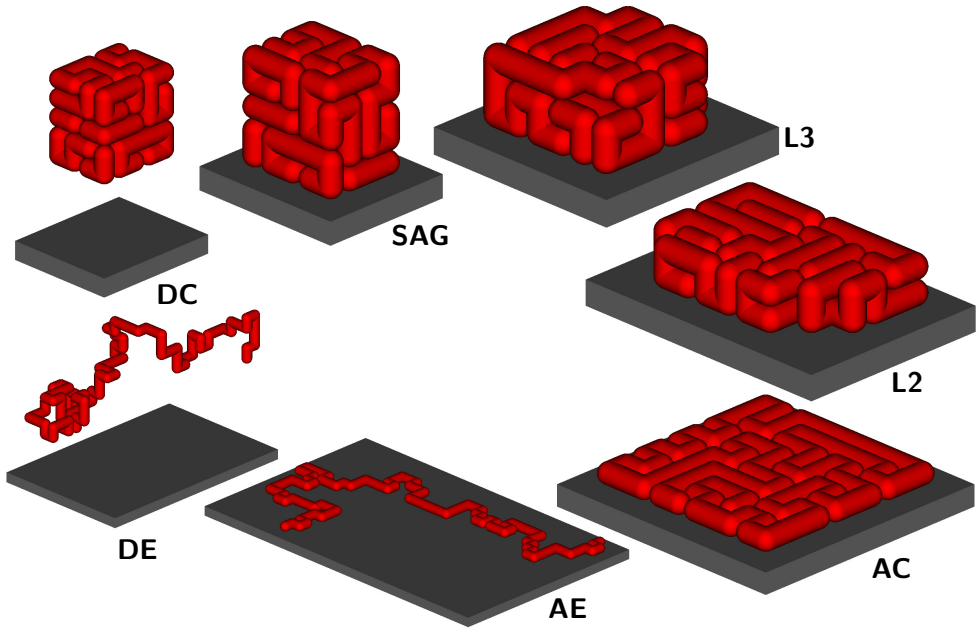

Figure 2: Representative conformations of the main pseudophases of a 100-bead homopolymer in a slit with one attractive surface. The polymer is represented as a tube with a diameter of the lattice spacing.

5. Specimen Results

We present briefly some results for a polymer of length $L = 100$, to illustrate the method. This type of system has been studied before, for example by chain growth [5], and the nomenclature used here is derived from that work. Representative conformations of the main pseudophases in a slit with one attractive surface are shown in Fig. 2. In the desorbed-collapsed (DC) and desorbed-expanded (DE) phases the polymer molecule is free from the attractive surface and adopts respectively globular and random coil conformations. The surface-attached globule (SAG) phase is essentially identical to DC, but rests on the surface. In the adsorbed-collapsed (AC) and adsorbed-expanded (AE) phases, all beads of the molecule reside on the surface, and two dimensional compact or random conformations are adopted, respectively. Finally L3 and L2 indicate pseudophases between the SAG and AC phases where the molecule adopts compact conformations of 3, and then 2 layers respectively.

In Fig. 3 the pseudophase diagram, represented as a contour map of heat capacity C, is shown for two situations: the raw results from a simulation in which the polymer is always in contact with the surface, determining $\mathbb{W}_1$, and the same results converted to slit geometry with a sterically confining wall at height $H = 200$.

It can be seen that the only significant difference is the elimination of the DC phase in the $\mathbb{W}_1$ case. The DE phase is still observed, but now conformations have a few surface contacts instead of moving completely free of the surface. This is unsurprising as it is clear that the three-dimensional random coil has greater entropy than the two-dimensional one, whereas there are no compact conformations with very few, but non-zero, surface contacts. A very low ridge in C is observed in the $\mathbb{W}_1$ case where the DC to SAG transition occurs in the slit; this indicates an orientation transition, now possible as the polymer molecule cannot desorb from the surface.

These results are broadly the same as those observed for tethered lattice polymers[22]. They may also be compared with the phase diagram for tethered chains of the bond-fluctuation model [12] and the slit system studied using multicanonical chain growth by [5]. The initial impression is that, above some minimum value, the slit width does not play a huge role in determining the broad features of the phase diagram, apart from the presence of the DC-SAG transition; this issue has been discussed by Möddel et al [15, 16].

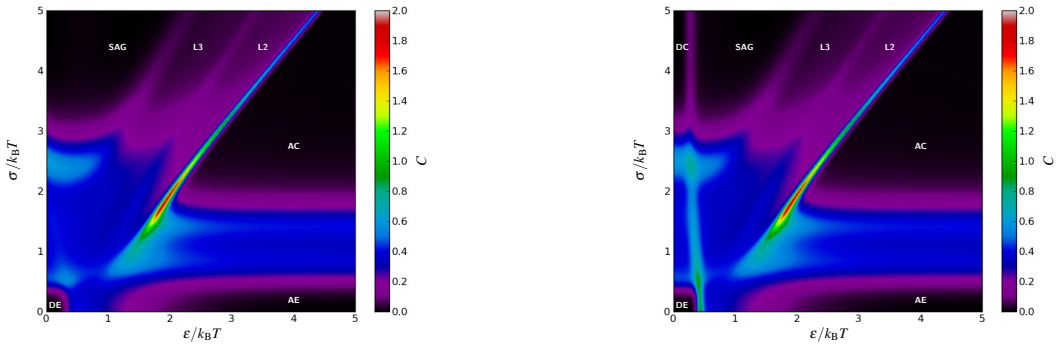

Figure 3: Specific heat C against internal (ϵ) and surface (σ) interaction strengths, both in units of k_BT, for a 100-bead homopolymer. Left: results of a $\mathbb{W}_1$ simulation, where the polymer is effectively always in contact with an attractive surface. Right: results converted to $\mathbb{W}_H$, corresponding to a polymer in a slit with one attractive surface and a second, sterically confining, surface at $H = 200$.

6. Discussion and Conclusions

This paper has shown explicitly how results for a simple lattice model of a single polymer, in confined "slit" geometry or when adsorbed at a single planar surface, may be obtained by Wang-Landau simulations which do not directly involve the walls. A single Wang-Landau simulation, determining the density of internal states of the polymer resolved by the numbers of internal contacts and lower surface beads, supplemented if necessary by a second simulation counting both upper and lower surface beads, is sufficient to determine all the relevant quantities. The only necessary assumption is that of nearest-neighbour interactions, although the method could be extended to include short-ranged interactions beyond nearest-neighbour.

The principal advantage of the approach proposed here is that it yields results for all slit heights H at once. In addition, conventional Wang-Landau simulation in slit geometry is likely to suffer from some inefficiencies, which this approach avoids. Firstly, no moves are ever rejected here due to 'overlap with the walls'. Secondly, the conventional approach will spend some fraction of its time simulating states with $s = 0$, desorbed from both walls, which is not strictly necessary, as the corresponding density of states $\mathbb{W}_0$ can be obtained from $\mathbb{W}_1$ or $\mathbb{W}_2$. Thirdly, any transition between the $s = 0$ state and any $s \neq 0$ state requires proximity of the chain and the wall: a molecule making a desorbed, diffusive, excursion in the slit will experience long intervals between opportunities to make such transitions, interrupted by long periods in the adsorbed state in which the overwhelming fraction of attempts to desorb will be rejected. A conventional Wang-Landau simulation would become very inefficient because of this, for large H.

We have investigated some ways of improving the efficiency of the basic method used here: for instance, there is nothing intrinsically unique about the z-direction, so any polymer move could be accompanied by a choice between different orientations relative to the surface, with the possibility of optimization. However, to date we have found no substantial speedup using this approach.

We have recently applied this technique to study the adsorption of lattice peptides on various patterned surfaces, and this will be the subject of a future publication [23].

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